Sarcosine, N-(3-methylbut-2-enoyl)-, heptadecyl ester

Inchi: InChI=1S/C25H47NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-29-25(28)22-26(

InchiKey: XYCOMDDXFKKOBW-UHFFFAOYSA-N

Formula: C25H47NO3

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C=C(C)C

Mol. weight [g/mol]: 409.65

Physical Properties

Property code	Value	Unit	Source
gf	-20.77	kJ/mol	Joback Method
hf	-741.75	kJ/mol	Joback Method
hfus	66.81	kJ/mol	Joback Method
hvap	89.23	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.826		Crippen Method
mcvol	377.800	ml/mol	McGowan Method
pc	838.21	kPa	Joback Method
rinpol	3137.00		NIST Webbook
rinpol	3137.00		NIST Webbook
tb	918.04	K	Joback Method
tc	1125.14	K	Joback Method
tf	507.03	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1265.90	J/mol×K	918.04	Joback Method
cpg	1286.52	J/mol×K	952.56	Joback Method
cpg	1305.88	J/mol×K	987.07	Joback Method
cpg	1324.05	J/mol×K	1021.59	Joback Method
cpg	1341.10	J/mol×K	1056.10	Joback Method
cpg	1357.12	J/mol×K	1090.62	Joback Method
cpg	1372.18	J/mol×K	1125.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321527&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume